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*Americium Thermodynamic Data  
for the EQ3/6 Database*

Los Alamos

Los Alamos National Laboratory  
Los Alamos, New Mexico 87545

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## **Americium Thermodynamic Data for the EQ3/6 Database**

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# AMERICIUM THERMODYNAMIC DATA FOR THE EQ3/6 DATABASE

by

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## ABSTRACT

Existing thermodynamic data for aqueous and solid species of americium have been reviewed and collected in a form that can be used with the EQ3/6 database. Data that are important in solubility calculations for americium at a proposed Yucca Mountain nuclear waste repository were emphasized. Conflicting data exist for americium complexes with carbonates. Essentially no data are available for americium solids or complexes at temperatures greater than 25°C.

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## I. INTRODUCTION

Americium is one of the radioactive waste elements that exists in spent fuel and reprocessed waste from nuclear reactors. Two isotopes of americium,  $^{241}\text{Am}$  and  $^{243}\text{Am}$ , are important radionuclides when considering geologic disposal of radioactive wastes.<sup>1</sup> For this reason, an understanding of the solubility and speciation of americium in aqueous solution will be necessary for geochemical modeling of a repository. At Los Alamos, the EQ3/6 chemical equilibrium computer programs are being used for geochemical modeling of Yucca Mountain, the proposed site being studied as part of the Nevada Nuclear Waste Storage Investigations.<sup>2</sup> No thermodynamic data for americium are currently available in the EQ3/6 database, but the literature has been reviewed and data are being collected and added to the database. This americium database will be used to:

- (1) assess the completeness and accuracy of existing thermodynamic data for americium,
- (2) estimate the solubility of americium in water at Yucca Mountain, and

- (3) guide future experimental work to answer important questions about americium behavior in aqueous solution.

## II. TYPES OF THERMODYNAMIC DATA NEEDED

The data needed for chemical equilibrium calculations are equilibrium constants for reactions that involve the species of interest and the aqueous basis species. However, thermodynamic data are usually not compiled in this way. A program that is part of the EQ3/6 program package (MCRT) can be used to convert basic thermodynamic data, such as free energies of formation, entropies, and heat capacities, into the data needed for equilibrium calculations.<sup>3</sup>

A minimum requirement for aqueous species is the free energy of formation of the species from the elements in their standard states at one temperature. Data usually exist at 25°C, and an equilibrium constant can be calculated at that temperature by using the free energy of formation information. If, in addition, the entropy of the species or the entropy or enthalpy change of a reaction forming the species is known at the same temperature, a number of extrapolation techniques can be used to calculate equilibrium-constant data for the aqueous species over the 0 to 300°C temperature range.

For solids too, the minimum required data are the free energy of formation of the species from the elements in their standard states at one temperature. This information can be used to calculate an equilibrium constant at that temperature. If heat capacity data or the enthalpy change for a reaction forming the species are also available, equilibrium constants can be determined at other temperatures.

## III. AMERICIUM DATA

In the literature, there are thermodynamic data for 26 aqueous species of americium. In addition, three other aqueous species that could be important have been postulated, but no thermodynamic data have been reported at this time. A listing of the species and accompanying data are contained in App. A, which is a copy of the input file MDAQS for the MCRT program. The file contains a list of references for the data and explains how specific data were chosen when conflicting sources were available. Emphasis was given to complexes of Am(III), which is the most likely oxidation state in dilute,

near-neutral solutions. Data were found for complexes of  $\text{Am}^{3+}$  with  $\text{OH}^-$ ,  $\text{CO}_3^{2-}$ ,  $\text{F}^-$ ,  $\text{Cl}^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{PO}_4^{3-}$ , and  $\text{NO}_3^-$ . At least one species in three other oxidation states ( $\text{Am}^{4+}$ ,  $\text{AmO}_2^+$ , and  $\text{AmO}_2^{2+}$ ) was also included.

Thermodynamic data were found for only three solids of americium that would likely precipitate from aqueous solution:  $\text{Am}(\text{OH})_3$ ,  $\text{Am}(\text{OH})\text{CO}_3$ , and  $\text{Am}_2(\text{CO}_3)_3$ . Solubility measurements have also been reported for solid  $\text{AmO}_2$ , but the authors did not report equilibrium-constant data. A listing of the species and accompanying data are contained in App. B, which is a copy of the input file MDSOL for the MCRT program. The file contains a list of references for the data and explains how specific data were chosen when conflicting sources were available.

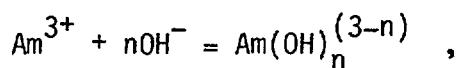
Appendix C contains a listing of the input file REAC for the MCRT program. REAC specifies the reactions involving the americium complexes and solids for which equilibrium constants will be determined by the MCRT program.

The output from the MCRT program is a file containing equilibrium-constant data for the reactions specified at 0, 25, 60, 100, 150, 200, 250, and 300°C. Appendix D contains a listing of this file, which also gives data for the species, the reaction being considered, and equilibrium constants as  $\log_{10}K$ . A value of 500 for  $\log_{10}K$  indicates that no data are available at that temperature.

#### IV. DISCUSSION

The americium data collected in this review have been examined in an attempt to discover any discrepancies or inconsistencies. This is particularly important when data from more than one source are available or when the choice of other thermodynamic data influences the results of a particular experimenter.

Data for three of the hydrolysis products of  $\text{Am}^{3+}$  [ $\text{Am}(\text{OH})_2^{2+}$ ,  $\text{Am}(\text{OH})_2^+$ , and  $\text{Am}(\text{OH})_3^-$ ] have been reported by a number of experimenters (see App. A references). A fourth hydrolysis product [ $\text{Am}(\text{OH})_4^-$ ] has been postulated by analogy with the rare earths, but no evidence for its existence has been published.<sup>4</sup> Figure 1 shows a plot of  $\log_{10}K$  for the reaction



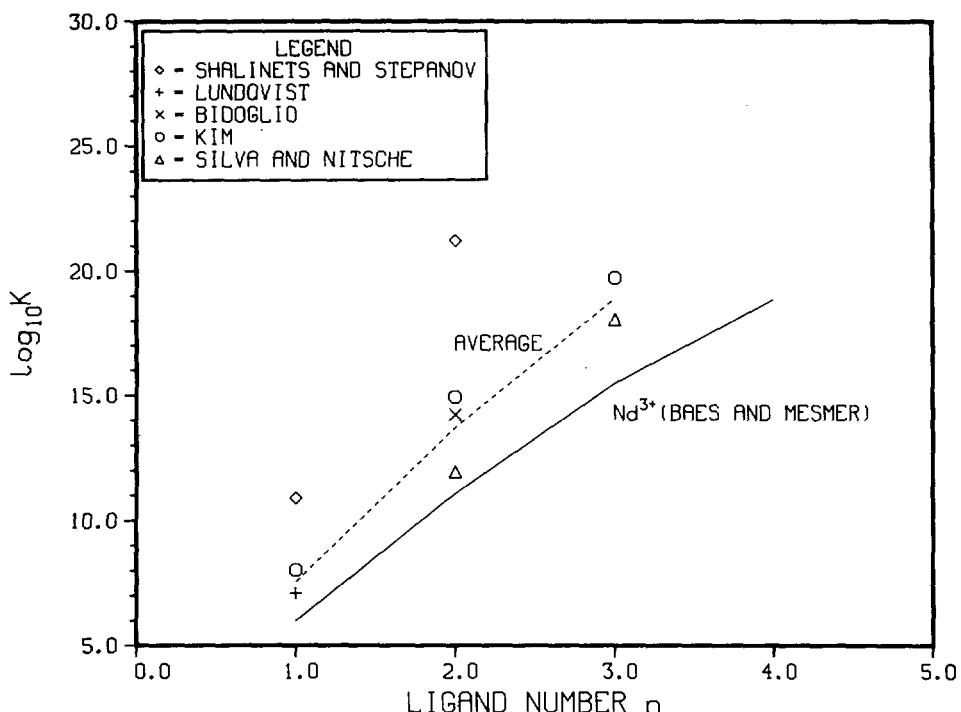


Fig. 1. Americium hydrolysis products.

as a function of the number of ligands  $n$ .<sup>5-9</sup> Three values have been shown for  $n = 1$ , four values for  $n = 2$ , and two values for  $n = 3$ . In addition, data for the analogous reaction for neodymium are shown.<sup>10</sup> The  $Nd^{3+}$  ion is often used as a chemical analogue for  $Am^{3+}$ . The americium complexes appear to be more stable (larger  $\log_{10} K$ ) than the comparable neodymium complexes. There was no clear reason to select the data of any one or two experimenters for these complexes; instead, average values were chosen and are shown by the dashed line in Fig. 1 (see comments in App. A for these species). In determining these average values, Shalinets and Stepanov's data for  $n = 1$  and  $n = 2$  were disregarded as being out of line with the other reported data.<sup>5</sup>

There have been two recent reports of the solubility of solid  $Am(OH)_3$ .<sup>8,11</sup> Calculating a solubility product for  $Am(OH)_3$  requires knowledge of the hydrolysis equilibria; values for formation constants of hydrolysis products must either be assumed or determined as part of the work. Thus, the resulting solubility product is related to the choice of hydrolysis equilibrium constants; if either the solubility product or hydrolysis equilibrium constants are varied independently, incorrect predictions of solubility can result. Thermodynamic

data for solid  $\text{Am(OH)}_3$  were chosen as intermediate between the values reported by Silva<sup>11</sup> and Kim<sup>8</sup> and were consistent with the choices of hydrolysis-product equilibrium constants described in the previous paragraph. Figure 2 shows the calculated solubility of solid  $\text{Am(OH)}_3$  compared with measured solubilities under the conditions of the two experimental measurements. Reported solubilities of americium from Edelstein<sup>12</sup> and Rai<sup>13</sup> are also shown; the identity of the solid phase controlling solubility was not determined in either of these experiments.

The solubility of solid  $\text{AmO}_2$  was also reported as a function of pH by Kim.<sup>8</sup> Dissolution of  $\text{AmO}_2$  involves the reduction of  $\text{Am}^{4+}$  to  $\text{Am}^{3+}$  and the formation of  $\text{Am}^{3+}$  complexes in solution. Thus, the solution Eh or some other measure of the redox state of the solution is necessary to interpret the solubility data in terms of equilibrium reactions. This work did not include redox measurements, so meaningful thermodynamic data cannot be derived from the solubility data.

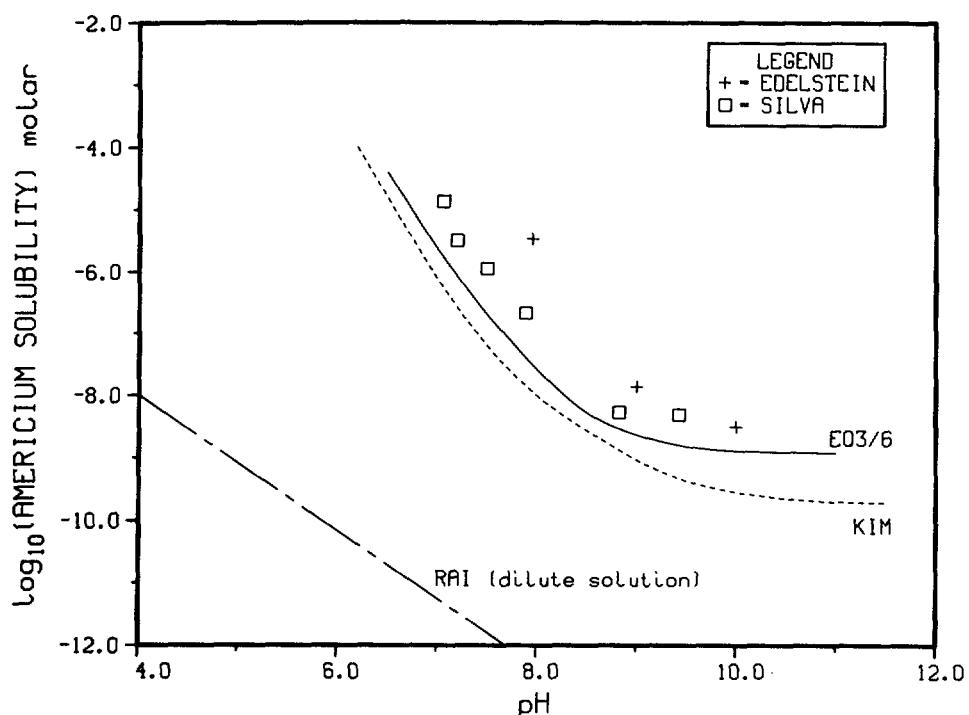


Fig. 2. Americium solubility in 0.1 M  $\text{NaClO}_4$  at 25°C.

Bidoglio<sup>6</sup> and Lundqvist<sup>7</sup> have experimentally determined complex formation between  $\text{Am}^{3+}$ ,  $\text{OH}^-$ , and carbonate species. This work has recently been reviewed by Newton and Sullivan.<sup>14</sup> The species identified in each work and their formation constants were used with the hydrolysis products of  $\text{Am}^{3+}$  (defined above) to calculate the predominant species in aqueous solution in the pH range from 6 to 11. Figure 3 shows the results for total carbonate of  $2 \times 10^{-3}$  M at ionic strength 0.1. These conditions are similar to the experimental conditions employed by the two investigators. It is apparent that the predominant species predicted from the two sets of formation constants are quite different.

Bidoglio should have seen evidence for the  $\text{AmCO}_3^+$  complex reported by Lundqvist, and Lundqvist should have observed the  $\text{AmHCO}_3^{2+}$  and  $\text{Am}(\text{HCO}_3)_2^+$  complexes reported by Bidoglio. In the range of interest for water at Yucca Mountain (pH 6 to 8), the Bidoglio data predict that  $\text{AmHCO}_3^{2+}$ ,  $\text{Am}(\text{HCO}_3)_2^+$ , and  $\text{Am}(\text{CO}_3)_2^-$  are the primary aqueous species, whereas the Lundqvist data predict that  $\text{Am}^{3+}$ ,  $\text{AmCO}_3^+$ ,  $\text{Am}(\text{CO}_3)_2^-$ , and two of the hydrolysis products ( $\text{AmOH}^{2+}$  and  $\text{Am}(\text{OH})_2^+$ ) predominate. At this time, there are no other sources of information that would verify either of these two conflicting sets of data. The Lundqvist data have been employed for further calculations with EQ3/6 (see App. A), but this should be considered as an interim choice that will probably be modified as more data become available.

Evidence has been reported for two solids of americium with carbonate,  $\text{Am(OH)}\text{CO}_3$  and  $\text{Am}_2(\text{CO}_3)_3$ . Silva and Nitsche<sup>9</sup> have recently reported a formation constant for solid  $\text{Am(OH)}\text{CO}_3$ ; they employed the complex formation constants of Lundqvist to analyze their data so their result was used directly. Their experiment was conducted at pH 6.1 and total carbonate of  $2 \times 10^{-4}$  M; neither of the carbonate complexes reported by Lundqvist is important under these conditions. If the carbonate complexes reported by Bidoglio had been used to analyze the data, significant aqueous concentrations of  $\text{AmHCO}_3^{2+}$  and  $\text{Am}(\text{HCO}_3)_2^+$  would exist under these conditions and the reported formation constant would be different. Shiloh et al.<sup>15</sup> reported evidence for the formation of solid  $\text{Am}_2(\text{CO}_3)_3$  at high carbonate concentrations and high pH. The reported solubility of this material was used to estimate a solubility product for the solid. This estimate should be considered speculative at this time.

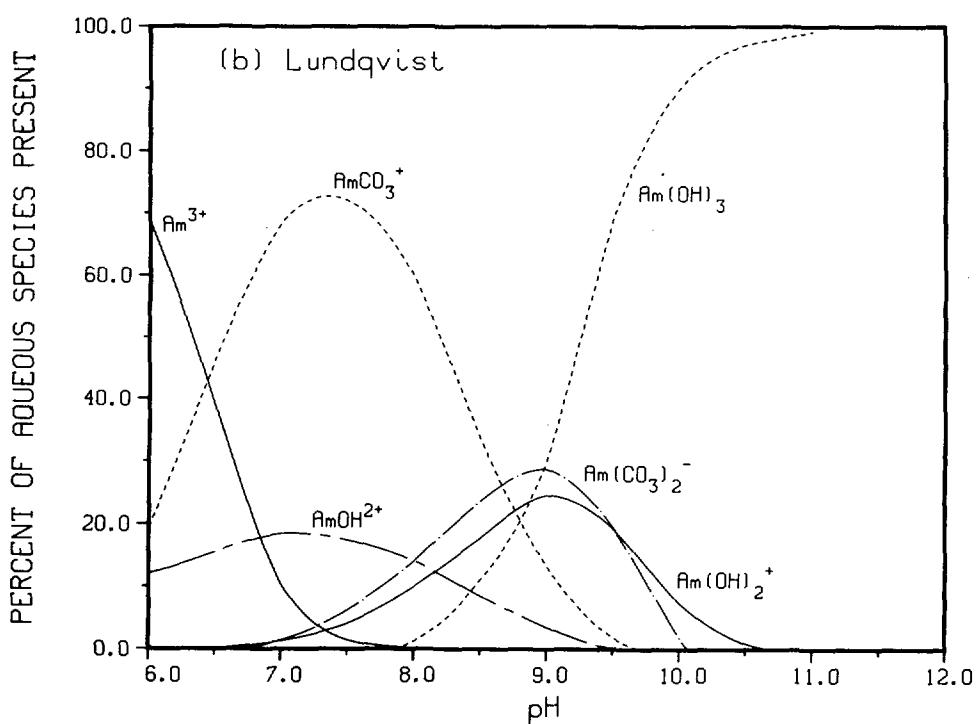
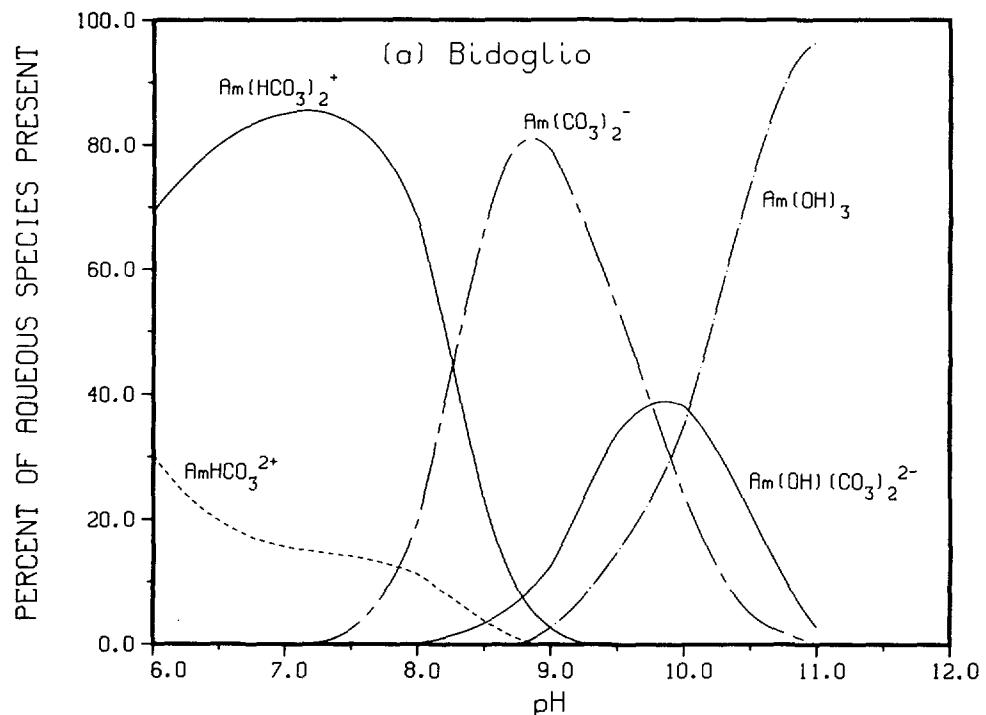


Fig. 3. Americium speciation in 0.1 M NaClO<sub>4</sub> at 25°C with  $2 \times 10^{-3}$  M total carbonate present.

Data for the formation of americium complexes with  $F^-$ ,  $Cl^-$ ,  $SO_4^{2-}$ ,  $PO_4^{3-}$ , and  $NO_3^-$  are also listed in App. A. Where possible, thermodynamic data for these complexes were taken from the review by Phillips.<sup>16</sup> Of these anions, only complexes with  $F^-$  appear to be of any importance in water at Yucca Mountain (see the following section). Formation constants for the fluoride complexes were taken from Phillips' review; they appear to be reliable data.

One aspect of essentially all the data collected for americium is that only 25°C data are available. For a thorough analysis of americium solubility, it may be necessary to extend data for important complexes and solids to higher temperatures.

## V. SOLUBILITY OF AMERICIUM IN WATER FROM YUCCA MOUNTAIN

The solubility of americium will influence its rate of transport from a repository along water flowpaths toward the accessible environment. Calculations of americium solubility in water from Yucca Mountain were done using EQ3/6 and the thermodynamic data listed in App. D. Analyses of water from Well J-13 at the Nevada Test Site were used to define the water composition.<sup>17</sup> The observed pH of Well J-13 water is approximately 7, and total carbonate is  $2.3 \times 10^{-3}$  M. The Eh was assumed to be 400 mV; this assumption should not affect the results because only the Am(III) oxidation state is expected in dilute, near-neutral solutions. It was assumed that the solid controlling solubility is  $Am(OH)CO_3$ . Figure 4 shows a plot of americium solubility and the predominant aqueous americium species from pH 6 to 8. At pH 6, a variety of species contribute to the aqueous americium content; at pH 7 to 8,  $AmCO_3^+$  is the predominant aqueous species. With Well J-13 water in this pH range, the hydrolysis products are not important aqueous species. Solid  $Am_2(CO_3)_3$  was also near saturation under these conditions. Although solid  $Am(OH)_3$  was undersaturated, it could control solubility at higher pH or at lower total carbonate.

## VI. RECOMMENDATIONS

This review has highlighted two problems with the available thermodynamic data that will be used to calculate americium solubility in aqueous solutions such as Well J-13 water. There is a conflict between the only two available sources of data for americium complexes with carbonate species. Because carbonate is the primary anion in water from Yucca Mountain, this conflict

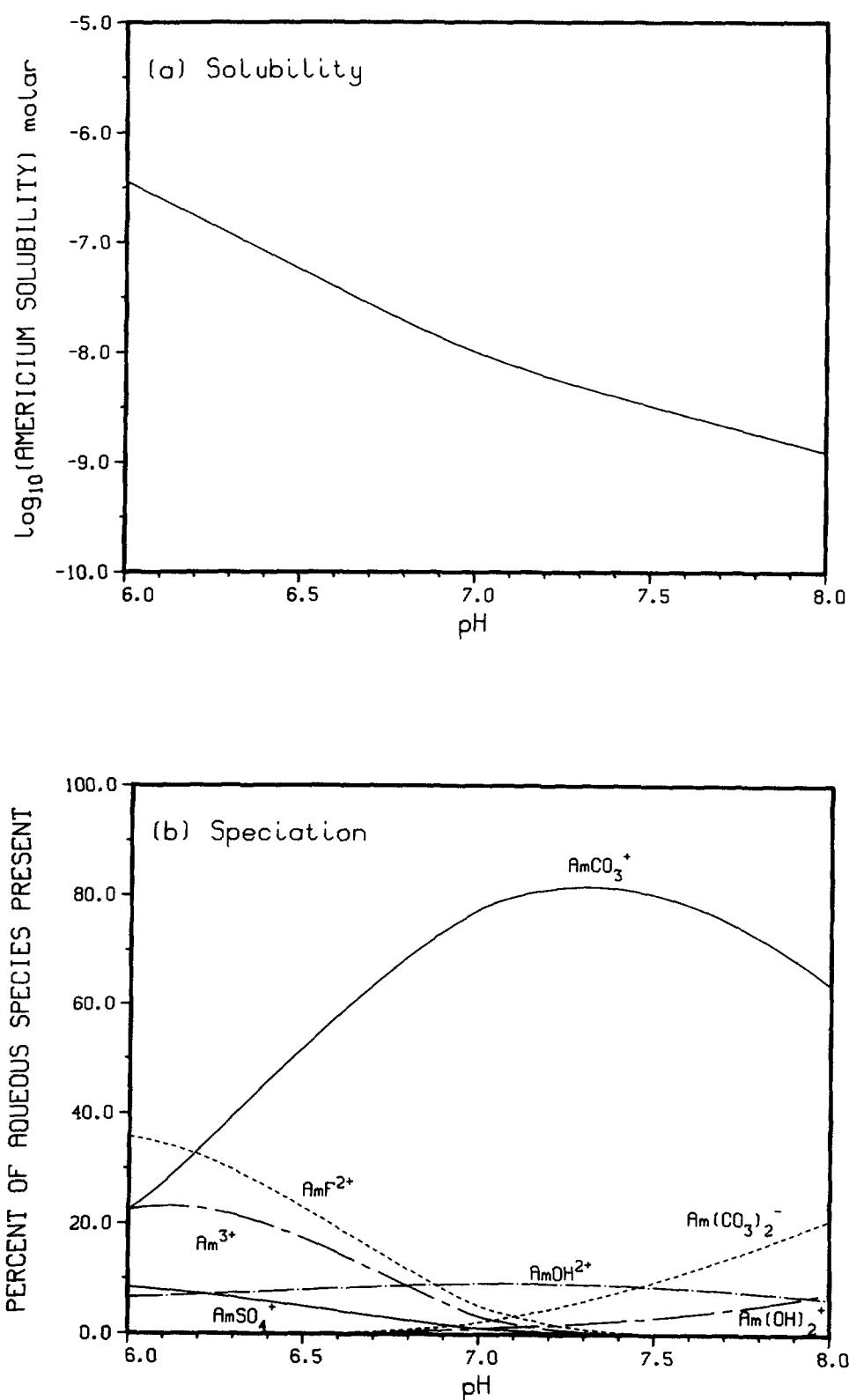


Fig. 4. Americium solubility and speciation in Well J-13 water at 25°C.

must be resolved before americium solubility and speciation can be accurately determined for performance assessment. Further experimental work is needed to (a) identify the stoichiometry of the predominant aqueous complexes of americium with carbonate and (b) determine their formation constants. The second problem is that only data at 25°C are available for most americium species and compounds. Higher temperature data are needed, especially for solids controlling solubility and predominant aqueous species.

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## APPENDIX A

Appendix A is a listing of the input file MDAQS for the MCRT program. This file contains thermodynamic data for aqueous species of americium.

MDAQSAM DATA FOR AQUEOUS COMPLEXES OF AMERICIUM (SEE BOTTOM OF FILE)  
LAST REVISED 10/07/83

AM+++

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
SOURCE= QUALITY=  
CHARGE= 4.0 TITR. FACTOR= 0.0 EQ/MOL  
ION TYPE= 1 ION SIZE= 0.0 A  
HYDR. NO.= O.O  
1 CHEMICAL ELEMENTS=  
1.000 AM  
TEMP= 298.150 K PRESS= 1.000 BARS  
DELGO= -89.200 KCAL/MOL DELHO= -103.300 KCAL/MOL  
SO= -97.000 CAL/MOL/K SE= 3.560 CAL/MOL/K  
VO= 0.000 CC/MOL  
CP= 0.000 CAL/MOL/K  
NO T-P DATA GRID  
O SPECIES IN REACTION=  
0.000 XX 0.000 XX 0.000 XX  
LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
DELSOR= 500.000 CAL/MOL/K

\*  
\* SE TAKEN SAME AS PU+++.  
\* FUGER AND DETTING (1976).  
+-----

AMO2+

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
SOURCE= QUALITY=  
CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
ION TYPE= 1 ION SIZE= 0.0 A  
HYDR. NO.= O.O  
2 CHEMICAL ELEMENTS=  
1.000 AM 2.000 O  
TEMP= 298.150 K PRESS= 1.000 BARS  
DELGO= -177.100 KCAL/MOL DELHO= -192.400 KCAL/MOL  
SO= -5.000 CAL/MOL/K SE= 2.180 CAL/MOL/K  
VO= 0.000 CC/MOL  
CP= 0.000 CAL/MOL/K  
NO T-P DATA GRID  
O SPECIES IN REACTION=  
0.000 XX 0.000 XX 0.000 XX  
LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
DELSOR= 500.000 CAL/MOL/K

\*  
\* SE FROM MCGLYNN AND SMITH (1961).  
\* FUGER AND DETTING (1976).  
+-----

AMO2++

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
SOURCE= QUALITY=  
CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL  
ION TYPE= 1 ION SIZE= 0.0 A  
HYDR. NO.= O.O  
2 CHEMICAL ELEMENTS=  
1.000 AM 2.000 O  
TEMP= 298.150 K PRESS= 1.000 BARS  
DELGO= -140.400 KCAL/MOL DELHO= -155.800 KCAL/MOL  
SO= -21.000 CAL/MOL/K SE= 4.570 CAL/MOL/K  
VO= 0.000 CC/MOL  
CP= 0.000 CAL/MOL/K  
NO T-P DATA GRID  
O SPECIES IN REACTION=  
0.000 XX 0.000 XX 0.000 XX  
LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
DELSOR= 500.000 CAL/MOL/K

\*  
\* SE FROM MCGLYNN AND SMITH (1961).  
\* FUGER AND DETTING (1976).  
+-----

AMOH++

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
SOURCE= QUALITY=  
CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL  
ION TYPE= O ION SIZE= 0.0 A  
HYDR. NO.= O.O  
3 CHEMICAL ELEMENTS=  
1.000 AM 1.000 O 1.000 H  
TEMP= 298.150 K PRESS= 1.000 BARS

```

DELGO= -191.12 KCAL/MOL   DELHO= 500.000 KCAL/MOL
      SO= 500.000 CAL/MOL/K    SE= 0.000 CAL/MOL/K
      VO= 0.000 CC/MOL
      CP= 0.000 CAL/MOL/K

NO T-P DATA GRID
O SPECIES IN REACTION=
  0.000 XX          0.000 XX          0.000 XX
    LOG K= 500.000     DELHOR= 500.000 KCAL/MOL
    DELSOR= 500.000 CAL/MOL/K

*
* LUNDQVIST (1982), LOG K = -7.50 FOR AM+++ + H2O = AMOH++ + H+ AT I = 1.
* KIM (1983A), LOG K = 8.03 FOR AM+++ + OH- = AMOH++ AT I = 0.
* SHALINETS AND STEPANOV (1972), LOG K = 10.7 FOR AM+++ + OH- =
* AMOH++ AT I = 0.005; DATA SEEMS OUT OF LINE WITH OTHERS.
* USE AVERAGE OF KIM AND LUNDQVIST CORRECTED TO I = 0.

```

AM(OH)2+  
 ENTERED BY= J.F. KERRISK DATE= 09/01/83  
 SOURCE= QUALITY=  
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 1 ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 2.000 O 2.000 H  
 TEMP= 298.150 K PRESS= 1.000 BARS  
 DELGO= -237.10 KCAL/MOL DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX 0.000 XX 0.000 XX  
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

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\* BIDOGLIO ET AL. (1983), LOG K = 12.845 FOR  $\text{AM}^{+++} + 2\text{OH}^- = \text{AM(OH)}_2^+$   
 \* AT I = 0.2.  
 \* SILVA (1982), LOG K = -16.7 FOR  $\text{AM}^{+++} + 2\text{H}_2\text{O} = \text{AM(OH)}_2^+ + 2\text{H}^+$  AT  
 \* I = 0.1.  
 \* KIM (1983A), LOG K = 14.93 FOR  $\text{AM}^{+++} + 2\text{OH}^- = \text{AM(OH)}_2^+$  AT I = 0.  
 \* SHALINETS AND STEPANOV (1972), LOG K = 20.9 FOR  $\text{AM}^{+++} + 2\text{OH}^- =$   
 \*  $\text{AM(OH)}_2^+$  AT I = 0.005; DATA SEEMS OUT OF LINE WITH OTHERS.  
 \* USE AVERAGE OF BIDOGLIO, SILVA, AND KIM DATA CORRECTED TO I = 0.

AM(OH)3  
 ENTERED BY= J.F. KERRISK DATE= 09/01/83  
 SOURCE= QUALITY=  
 CHARGE= 0.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= O ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 3.000 O 3.000 H  
 TEMP= 298.150 K PRESS= 1.000 BARS  
 DELGO= -281.770 KCAL/MOL DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX 0.000 XX 0.000 XX  
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

+-----  
 AMCO3+  
 ENTERED BY= J.F. KERRISK DATE= 09/01/83  
 SOURCE= QUALITY=  
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 1 ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
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 1.000 AM 3.000 O 1.000 C  
 TEMP= 298.150 K PRESS= 1.000 BARS  
 DELGO= -279.81 KCAL/MOL DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL

CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX 0.000 XX 0.000 XX  
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\* LUNDQVIST (1982), LOG K = 5.81 FOR AM+++ + CO3-- = AMC03+ AT I = 1.0.  
 +-----  
 AM(CO3)2-  
 ENTERED BY= J.F. KERRISK DATE= 09/01/83  
 SOURCE= QUALITY=  
 CHARGE= -1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 3 ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 6.000 O 2.000 C  
 TEMP= 298.150 K PRESS= 1.000 BARS  
 DELGO= -412.14 KCAL/MOL DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX 0.000 XX 0.000 XX  
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\* BIDOGLIO ET AL. (1983), LOG K = 11.45 FOR AM+++ + 2CO3-- = AM(CO3)2-  
 \* AT I = 0.2.  
 \* LUNDQVIST (1983), LOG K = 9.72 FOR AM+++ + 2CO3-- = AM(CO3)2-  
 \* AT I = 1.0.  
 \* USE LUNDQVIST VALUE CORRECTED TO I = 0.  
 +-----  
 AM(CO3)3---  
 ENTERED BY= J.F. KERRISK DATE= 09/01/83  
 SOURCE= QUALITY=  
 CHARGE= -3.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 3 ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 3.000 C 9.000 O  
 TEMP= 298.150 K PRESS= 1.000 BARS  
 DELGO= 500.000 KCAL/MOL DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX 0.000 XX 0.000 XX  
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\* EVIDENCE FOR EXISTANCE FROM KIM (1983B), BUT NO PUBLISHED DATA.  
 \* EVIDENCE OF RARE EARTH TRICARBONATE FROM FERRI ET AL. (1983), BUT  
 \* NO DATA FOR AMERICIUM.  
 +-----  
 AM(OH)CO3  
 ENTERED BY= J.F. KERRISK DATE= 09/01/83  
 SOURCE= QUALITY=  
 CHARGE= 0.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= O ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 4 CHEMICAL ELEMENTS=  
 1.000 AM 4.000 O 1.000 H  
 1.000 C  
 TEMP= 298.150 K PRESS= 1.000 BARS  
 DELGO= 500.000 KCAL/MOL DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX 0.000 XX 0.000 XX  
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\* EVIDENCE FOR EXISTANCE FROM KIM (1983B), BUT NO PUBLISHED DATA.  
 +-----  
 AM(OH)(CO3)2--

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
 SOURCE= QUALITY=  
 CHARGE= -2.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 3 ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 4 CHEMICAL ELEMENTS=  
 1.000 AM 1.000 H 7.000 O  
 2.000 C  
 TEMP= 298.150 K PRESS= 1.000 BARS  
 DELGO= 500.000 KCAL/MOL DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX 0.000 XX 0.000 XX  
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\* EVIDENCE FOR EXISTANCE FROM KIM (1983B), BUT NO PUBLISHED DATA.  
 \* BIDOGGLIO ET AL. (1983), LOG K = 15.57 FOR  
 \* AM++ + OH- + 2CO3-- = AM(OH)(CO3)2-- AT I = 0.2.  
 \* DELGO = -457.00 KCAL/MOL: NOT USED IN DATAO AT THIS TIME.  
 -----

AM(OH)2CO3-  
 ENTERED BY= J.F. KERRISK DATE= 09/01/83  
 SOURCE= QUALITY=  
 CHARGE= -1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 3 ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 4 CHEMICAL ELEMENTS=  
 1.000 AM 5.000 O 2.000 H  
 1.000 C  
 TEMP= 298.150 K PRESS= 1.000 BARS  
 DELGO= 500.000 KCAL/MOL DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX 0.000 XX 0.000 XX  
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\* EVIDENCE FOR EXISTANCE FROM KIM (1983B), BUT NO PUBLISHED DATA.  
 -----

AMHC03++  
 ENTERED BY= J.F. KERRISK DATE= 09/01/83  
 SOURCE= QUALITY=  
 CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 1 ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 4 CHEMICAL ELEMENTS=  
 1.000 AM 1.000 H 1.000 C  
 3.000 O  
 TEMP= 298.150 K PRESS= 1.000 BARS  
 DELGO= 500.000 KCAL/MOL DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX 0.000 XX 0.000 XX  
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\* BIDOGGLIO ET AL. (1983), LOG K = 4.79 FOR AM++ + HC03- = AMHC03++ AT  
 \* I = 0.2.  
 \* DELGO = -291.14 KCAL/MOL; NOT USED IN DATAO AT THIS TIME.  
 -----

AM(HC03)2+  
 ENTERED BY= J.F. KERRISK DATE= 09/01/83  
 SOURCE= QUALITY=  
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 1 ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 4 CHEMICAL ELEMENTS=  
 1.000 AM 2.000 H 2.000 C  
 6.000 O  
 TEMP= 298.150 K PRESS= 1.000 BARS

DELGO= 500.000 KCAL/MOL    DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K    SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX                0.000 XX                0.000 XX  
 LOG K= 500.000            DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\*  
 \* BIDOGGLIO ET AL. (1983), LOG K = 8.15 FOR AM+++ + 2HC03- = AM(HC03)2+  
 \* AT I = 0.2.  
 \* DELGO = -436.75 KCAL/MOL; NOT USED IN DATA0 AT THIS TIME.  
 +-----  
**AMF++**  
 ENTERED BY= J.F. KERRISK                            DATE= 09/01/83  
 SOURCE=    QUALITY=  
 CHARGE= 2.0    TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 1    ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 2 CHEMICAL ELEMENTS=  
 1.000 AM                1.000 F  
 TEMP= 298.150 K                                    PRESS= 1.000 BARS  
 DELGO= -216.390 KCAL/MOL                        DELHO= 500.000 KCAL/MOL  
 SO= -25.9 CAL/MOL/K                              SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX                0.000 XX                0.000 XX  
 LOG K= 500.000            DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\*  
 \* AZIZ AND LYLE (1969).  
 \* PHILLIPS (1982) LOG K = 4.3 FOR AM+++ + F- = AMF++ AT I = 0.  
 \* SO FROM CHOPPIN AND UNREIN (1976), ERROR IN PAPER.  
 +-----  
**AMF2+**  
 ENTERED BY= J.F. KERRISK                            DATE= 09/01/83  
 SOURCE=    QUALITY=  
 CHARGE= 1.0    TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 1    ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 2 CHEMICAL ELEMENTS=  
 1.000 AM                2.000 F  
 TEMP= 298.150 K                                    PRESS= 1.000 BARS  
 DELGO= -287.940 KCAL/MOL                        DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K                            SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX                0.000 XX                0.000 XX  
 LOG K= 500.000            DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\*  
 \* AZIZ AND LYLE (1969).  
 \* PHILLIPS (1982), LOG K = 7.4 FOR AM+++ + 2F- = AMF2+ AT I = 0.  
 +-----  
**AMF3**  
 ENTERED BY= J.F. KERRISK                            DATE= 09/01/83  
 SOURCE=    QUALITY=  
 CHARGE= 0.0    TITR. FACTOR= 0.0 EQ/MOL  
 ION TYPE= 0    ION SIZE= 0.0 A  
 HYDR. NO.= 0.0  
 2 CHEMICAL ELEMENTS=  
 1.000 AM                3.000 F  
 TEMP= 298.150 K                                    PRESS= 1.000 BARS  
 DELGO= -359.630 KCAL/MOL                        DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K                            SE= 0.000 CAL/MOL/K  
 VO= 0.000 CC/MOL  
 CP= 0.000 CAL/MOL/K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX                0.000 XX                0.000 XX  
 LOG K= 500.000            DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K

\*  
 \* AZIZ AND LYLE (1969).  
 \* PHILLIPS (1982), LOG K = 10.6 FOR AM+++ + 3F- = AMF3 AT I = 0.

```

+-----+
AMCL++
ENTERED BY= J.F. KERRISK DATE= 09/01/83
  SOURCE= QUALITY=
  CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL
  ION TYPE= 1 ION SIZE= 0.0 A
  HYDR. NO.= 0.0
2 CHEMICAL ELEMENTS=
  1.000 AM 1.000 CL
    TEMP= 298.150 K PRESS= 1.000 BARS
    DELGO= -176.080 KCAL/MOL DELHO= 500.000 KCAL/MOL
    SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
    VO= 0.000 CC/MOL
    CP= 0.000 CAL/MOL/K
NO T-P DATA GRID
O SPECIES IN REACTION=
  0.000 XX 0.000 XX 0.000 XX
  LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
  DELSOR= 500.000 CAL/MOL/K
*
* WARD AND WELCH (1956).
* PHILLIPS (1982), LOG K = 1.1 FOR AM+++ + CL- = AMCL++ AT I = 0.
+-----+
AMCL2+
ENTERED BY= J.F. KERRISK DATE= 09/01/83
  SOURCE= QUALITY=
  CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL
  ION TYPE= 1 ION SIZE= 0.0 A
  HYDR. NO.= 0.0
2 CHEMICAL ELEMENTS=
  1.000 AM 2.000 CL
    TEMP= 298.150 K PRESS= 1.000 BARS
    DELGO= -208.09 KCAL/MOL DELHO= 500.000 KCAL/MOL
    SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
    VO= 0.000 CC/MOL
    CP= 0.000 CAL/MOL/K
NO T-P DATA GRID
O SPECIES IN REACTION=
  0.000 XX 0.000 XX 0.000 XX
  LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
  DELSOR= 500.000 CAL/MOL/K
*
* KHOPKAR AND NARAYANANKUTTY (1971)
* LOG K = 0.03 FOR AM+++ + 2CL- = AMCL2+ AT I = 1.
+-----+
AMSO4+
ENTERED BY= J.F. KERRISK DATE= 09/01/83
  SOURCE= QUALITY=
  CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL
  ION TYPE= 1 ION SIZE= 0.0 A
  HYDR. NO.= 0.0
3 CHEMICAL ELEMENTS=
  1.000 AM 4.000 O 1.000 S
    TEMP= 298.150 K PRESS= 1.000 BARS
    DELGO= -326.060 KCAL/MOL DELHO= 500.000 KCAL/MOL
    SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
    VO= 0.000 CC/MOL
    CP= 0.000 CAL/MOL/K
NO T-P DATA GRID
O SPECIES IN REACTION=
  0.000 XX 0.000 XX 0.000 XX
  LOG K= 500.000 DELHOR= 500.000 KCAL/MOL
  DELSOR= 500.000 CAL/MOL/K
*
* AZIZ ET AL. (1968).
* PHILLIPS (1982), LOG K = 3.6 FOR AM+++ + SO4-- = AMSO4+ AT I = 0.
+-----+
AM(SO4)2-
ENTERED BY= J.F. KERRISK DATE= 09/01/83
  SOURCE= QUALITY=
  CHARGE= -1.0 TITR. FACTOR= 0.0 EQ/MOL
  ION TYPE= 3 ION SIZE= 0.0 A
  HYDR. NO.= 0.0
3 CHEMICAL ELEMENTS=
  1.000 AM 8.000 O 2.000 S
    TEMP= 298.150 K PRESS= 1.000 BARS
    DELGO= -505.920 KCAL/MOL DELHO= 500.000 KCAL/MOL
    SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K
    VO= 0.000 CC/MOL
    CP= 0.000 CAL/MOL/K

```

NO T-P DATA GRID  
O SPECIES IN REACTION= 0.000 XX 0.000 XX 0.000 XX  
LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
DELSOR= 500.000 CAL/MOL/K

\*  
\* AZIZ ET AL. (1968).  
\* PHILLIPS (1982), LOG K = 5.0 FOR AM+++ + 2SO4-- = AM(SO4)2- AT I = 0.  
+-----

AMH2PO4++

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
SOURCE= QUALITY=  
CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL  
ION TYPE= 1 ION SIZE= 0.0 A  
HYDR. NO.= 0.0  
4 CHEMICAL ELEMENTS= 1.000 AM 4.000 D 1.000 P  
2.000 H TEMP= 298.150 K PRESS= 1.000 BARS  
DELGO= -417.090 KCAL/MOL DELHO= 500.000 KCAL/MOL  
SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
VO= 0.000 CC/MOL  
CP= 0.000 CAL/MOL/K

NO T-P DATA GRID  
O SPECIES IN REACTION= 0.000 XX 0.000 XX 0.000 XX  
LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
DELSOR= 500.000 CAL/MOL/K

\*  
\* LEBEDEV ET AL. (1979) LOG K = 2.73 FOR  
\* AM+++ + H2PO4- = AMH2PO4++ AT I = 0.  
+-----

AM(H2PO4)2+

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
SOURCE= QUALITY=  
CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
ION TYPE= 1 ION SIZE= 0.0 A  
HYDR. NO.= 0.0  
4 CHEMICAL ELEMENTS= 1.000 AM 8.000 D 2.000 P  
4.000 H TEMP= 298.150 K PRESS= 1.000 BARS  
DELGO= -688.610 KCAL/MOL DELHO= 500.000 KCAL/MOL  
SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
VO= 0.000 CC/MOL  
CP= 0.000 CAL/MOL/K

NO T-P DATA GRID  
O SPECIES IN REACTION= 0.000 XX 0.000 XX 0.000 XX  
LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
DELSOR= 500.000 CAL/MOL/K

\*  
\* LEBEDEV ET AL. (1979) LOG K = 3.72 FOR  
\* AM+++ + 2H2PO4- = AM(H2PO4)2+ AT I = 0.  
+-----

AM(H2PO4)3

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
SOURCE= QUALITY=  
CHARGE= 0.0 TITR. FACTOR= 0.0 EQ/MOL  
ION TYPE= 0 ION SIZE= 0.0 A  
HYDR. NO.= 0.0  
4 CHEMICAL ELEMENTS= 1.000 AM 12.000 D 3.000 P  
6.000 H TEMP= 298.150 K PRESS= 1.000 BARS  
DELGO= -960.11 KCAL/MOL DELHO= 500.000 KCAL/MOL  
SO= 500.000 CAL/MOL/K SE= 0.000 CAL/MOL/K  
VO= 0.000 CC/MOL  
CP= 0.000 CAL/MOL/K

NO T-P DATA GRID  
O SPECIES IN REACTION= 0.000 XX 0.000 XX 0.000 XX  
LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
DELSOR= 500.000 CAL/MOL/K

\*  
\* MOSKVIN (1971) LOG K = 2.85 FOR  
\* AM+++ + 3H2PO4- = AM(H2PO4)3 AT I = 1.  
+-----

AM(H2PO4)4-

ENTERED BY= J.F. KERRISK DATE= 09/01/83



```

O SPECIES IN REACTION=
 0.000 XX          0.000 XX          0.000 XX
  LOG K=      500.000    DELHOR=     500.000 KCAL/MOL
  DELSOR=   500.000 CAL/MOL/K

*
* MOSKVIN AND POZNYAKOV (1979) LOG K =
* AM02+ + HCO3 = AM02HCO3 AT I = 0.25.
+-----+
STOP.
MDAQSAM

```

#### DATA ON AQUEOUS COMPLEXES OF MANGANESE

##### NOTATION--

- DELGO = GIBBS ENERGY OF FORMATION
- DELGOR = GIBBS ENERGY OF REACTION
- DELHO = ENTHALPY OF FORMATION
- DELHOR = ENTHALPY OF REACTION
- SO = CONVENTIONAL ENTROPY
- SE = INTERNAL ELECTRONIC ENTROPY
- DELSOR = ENTROPY OF REACTION

NOTE THAT "500." IS ENTERED TO MEAN "NO DATA" FOR DELGO, DELHO, SO, LOG K, DELHO, AND DELSOR. NEVER ENTER ZERO OR LEAVE BLANK FOR THESE PARAMETERS UNLESS YOU MEAN TO USE AN ACTUAL VALUE OF ZERO.

IONIC STRENGTH CORRECTIONS NOTED IN THE ABOVE COMMENTS ON SPECIFIC SPECIES WERE MADE USING THE DAVIES EQUATION IN THE FORM

$$\text{LOG}(\text{GAMMA}) = 0.51 * (\text{Z}^{\star 2}) * ((\text{SQRT}(\text{I}) / (1 + \text{SQRT}(\text{I}))) - (0.2 * \text{I}))$$

WHERE GAMMA IS THE ACTIVITY COEFFICIENT, Z IS THE CHARGE, AND I IS THE IONIC STRENGTH.

#### DATA FOR AQUEOUS SPECIES=

NAME= AN ALPHABETIC OR ALPHANUMERIC STRING  
ENTERED BY= NAME OF PERSON WHO ENTERED DATA OR LAST REVISED IT  
DATE= DATA OF ENTERING OR REVISING DATA  
SOURCE= ALPHANUMERIC STRING IDENTIFYING A MAJOR SOURCE OF DATA. USE  
"SEE BELOW" FOR MINOR SOURCES  
QUALITY= ALPHANUMERIC STRING DESCRIBING THE PROBABLE ERROR IN GIBBS ENERGY  
OR ITS EQUIVALENT, BASED ON SUBJECTIVE JUDGEMENT AND CHOSEN FROM  
AMONG THE FOLLOWING (IN ORDER OF INCREASING VALUE)  
 BAD - DEMONSTRABLY BAD DATA- DO NOT USE EXCEPT IN ILLUSTRATIVE  
CALCULATIONS  
 POOR - LIKELY ERROR EXCEEDS A COUPLE OF KCAL OR SEVERAL KJ  
 RESTRICTED - AD HOC FIT TO A PARTICULAR SITUATION; SEE NOTES  
 SPECULATIVE - SPECIES NOT SHOWN CONCLUSIVELY TO EXIST  
 UNCERTAIN - CHOSEN RATHER ARBITRARILY FROM DIVERGENT REPORTED  
VALUES  
UNSPECIFIED - NO QUALITY INFORMATION  
(BLANK) - EQUIVALENT TO UNSPECIFIED  
FAIR - LIKELY ERROR LESS THAN A COUPLE OF KCAL OR A FEW KJ  
GOOD - LIKELY ERROR LESS THAN ABOUT ONE KCAL OR FOUR KJ  
THE CODE MUST BE MODIFIED TO ALLOW OTHER QUALITY PARAMETER INPUTS.  
UNRECOGNIZED INPUTS ARE SET TO "ERROR". DATA FOR WHICH THE QUALITY  
IS "RESTRICTED", "SPECULATIVE", OR "UNCERTAIN" MAY NUMERICALLY BE  
"FAIR" TO "GOOD". THE MAJOR UNCERTAINTY ASSOCIATED WITH THESE VALUES  
IS QUALITATIVE (I.E., UNCERTAINTY OF INTERPRETATION). DATA FOR WHICH  
THE QUALITY IS "POOR" MAY BE QUITE SUFFICIENT FOR MAKING "GOOD"  
CALCULATIONS- THIS DEPENDS ON THE SENSITIVITY OF THE RESULTS TO IT IN  
ANY PARTICULAR APPLICATION.  
CHARGE= ELECTRICAL CHARGE  
TITRATION FACTOR= WEIGHTING FACTOR FOR PH 4.5 (METHYL ORANGE)  
ALKALINITY  
ION TYPE= CRISS-COBBLE ION TYPE  
 0 NEUTRAL COMPLEX (MAY BE LEFT BLANK)  
 1 CATION (MAY BE LEFT BLANK)  
 2 SIMPLE ANION (MAY BE LEFT BLANK)  
 3 OXYANION  
 4 ACID OXYANION  
ION SIZE= DEBYE-HUCKEL HYDRATED ION SIZE (FOR ACTIVITY COEFFICIENT  
ESTIMATION)  
HYDRATION NUMBER= NUMBER OF BOUND WATER MOLECULES NOT EXPLICITLY  
SHOWN IN THE ASSUMED MOLECULAR FORMULA (FOR ACTIVITY COEFFICIENT

ESTIMATION)

TEMP= THE BASE POINT TEMPERATURE (K), USUALLY 298.15 K  
PRESS= THE BASE POINT PRESSURE (BARS), USUALLY 1 BAR

DELGO= THE APPARENT STANDARD PARTIAL MOLAL GIBBS ENERGY AT THE  
BASE POINT

DELHO= THE APPARENT STANDARD PARTIAL MOLAL ENTHALPY AT THE BASE POINT  
SO= THE CONVENTIONAL ENTRDPY AT THE BASE POINT

SE= THE INTERNAL ELECTRONIC ENTROPY; THIS FUNCTION IS ZERO EXCEPT FOR  
SOME ACTINIDE AND RARE EARTH SPECIES (IT IS USED IN CRISS-COBLE  
METHOD TEMPERATURE EXTRAPOLATIONS)

VO= THE PARTIAL MOLAL VOLUME AT THE BASE POINT; THERE IS NO CURRENT  
PROVISION FOR USING THIS INPUT IN THE CURRENT MCRT (AS OF 12/16/82)

CP= THE PARTIAL MOLAL HEAT CAPACITY AT THE BASE POINT; THERE IS NO  
CURRENT PROVISION FOR USING THIS INPUT IN THE CURRENT MCRT (AS OF  
12/16/82)

LOG K= LOG OF THE EQUILIBRIUM CONSTANT OF THE GIVEN REACTION AT THE  
BASE POINT

DELHOR= ENTHALPY OF THE GIVEN REACTION AT THE BASE POINT

DELSOR= ENTROPY OF THE GIVEN REACTION AT THE BASE POINT

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STOP.

## APPENDIX B

Appendix B contains a listing of the input file MDSOL for the MCRT program. This file contains thermodynamic data for solid species of americium.

MDSOLAM DATA FOR SOLIDS OF AMERICIUM (SEE BOTTOM OF FILE)  
LAST REVISED 10/07/83

-----  
AM(OH)3(C)

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
SOURCE= QUALITY=  
3 CHEMICAL ELEMENTS= 1.000 AM 3.000 O 3.000 H  
TEMP= 298.150 K PRESS= 1.000 BARS  
DELGO= -293.94 KCAL/MOL DELHO= 500.000 KCAL/MOL  
SO= 500.000 CAL/MOL/K VO= 0.000 CC/MOL  
1 HEAT CAPACITY RANGE(S) FOLLOW  
EQUATION= O CP OR A= 0.000 CAL/MOL/K  
B= 0.000 C= 0.000  
D= 0.000 E= 0.000  
LIMIT= 1000.000 K  
NO T-P DATA GRID  
O SPECIES IN REACTION= 0.000 XX 0.000 XX 0.000 XX  
LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
DELSOR= 500.000 CAL/MOL/K

\* KIM (1983A), LOG K = 28.56 FOR AM+++ + 3OH- = AM(OH)3(C) AT I = 0.  
\* SILVA (1982), LOG K = -16.6 FOR AM+++ + 3H2O = AM(OH)3(C) + 3H+  
\* AT I = 0.1.  
\* EDELSTEIN (1983), MEASURED SOLUBILITY OF SOLID THAT MAY HAVE BEEN  
\* AM(OH)3; SOLID PHASE NOT IDENTIFIED.  
\* USE DATA FROM KIM AND SILVA IN COMBINATION WITH ASSUMED HYDROLYSIS  
\* PRODUCT CONSTANTS FROM MDAQSAM FILE TO MATCH SOLUBILITY.  
\* LOG K = 27.8 FOR AM+++ + 3OH- = AM(OH)3(C) AT I = 0.

-----

AM(OH)CO3(C)

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
SOURCE= QUALITY=  
4 CHEMICAL ELEMENTS= 1.000 AM 1.000 C 1.000 H  
4.000 O  
TEMP= 298.150 K PRESS= 1.000 BARS  
DELGO= -338.04 KCAL/MOL DELHO= 500.000 KCAL/MOL  
SO= 500.000 CAL/MOL/K VO= 0.000 CC/MOL  
1 HEAT CAPACITY RANGE(S) FOLLOW  
EQUATION= O CP OR A= 0.000 CAL/MOL/K  
B= 0.000 C= 0.000  
D= 0.000 E= 0.000  
LIMIT= 1000.000 K  
NO T-P DATA GRID  
O SPECIES IN REACTION= 0.000 XX 0.000 XX 0.000 XX  
LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
DELSOR= 500.000 CAL/MOL/K

\* SILVA AND NITSCHE (1983), LOG K = -2.67 FOR AM+++ + HC03- + H2O =  
\* AM(OH)CO3(C) + 2H+ AT I = 0.1.  
\* KIM (1983B) HAS PROPOSED THIS SOLID ALSO, BUT NO DATA PUBLISHED.  
\* USE DATA FROM SILVA AND NITSCHE CORRECTED TO I = 0.

-----

AM2(CO3)3(C)

ENTERED BY= J.F. KERRISK DATE= 09/01/83  
SOURCE= QUALITY=  
3 CHEMICAL ELEMENTS= 2.000 AM 3.000 C 9.000 D  
TEMP= 298.150 K PRESS= 1.000 BARS  
DELGO= -716.100 KCAL/MOL DELHO= 500.000 KCAL/MOL  
SO= 500.000 CAL/MOL/K VO= 0.000 CC/MOL  
1 HEAT CAPACITY RANGE(S) FOLLOW  
EQUATION= O CP OR A= 0.000 CAL/MOL/K  
B= 0.000 C= 0.000  
D= 0.000 E= 0.000  
LIMIT= 1000.000 K  
NO T-P DATA GRID  
O SPECIES IN REACTION= 0.000 XX 0.000 XX 0.000 XX  
LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
DELSOR= 500.000 CAL/MOL/K

\* SHILOH ET AL. (1969) MEASURED SOLUBILITY OF AMERICIUM IN HIGH  
\* CARBONATE SOLUTIONS AND POSTULATED THIS SOLID PRECIPITATE.  
\* DATA ESTIMATED FROM THIER SOLUBILITY MEASUREMENTS.

\* LOG K = 37.5 FOR 2AM+++ + 3CO3-- = AM2(CO3)3(C)  
 \* IDENTITY OF SOLID AND DATA ARE SPECULATIVE.  
 +-----  
 AM02(C)  
 ENTERED BY= J.F. KERRISK DATE= 10/07/83  
 SOURCE= QUALITY=  
 2 CHEMICAL ELEMENTS=  
 1.000 AM 2.000 O  
 TEMP= 298.150 K PRESS= 1.000 BARS  
 DELGO= 500.000 KCAL/MOL DELHO= 500.000 KCAL/MOL  
 SO= 500.000 CAL/MOL/K VO= 0.000 CC/MOL  
 1 HEAT CAPACITY RANGE(S) FOLLOW  
 EQUATION= O CP OR A= 0.000 CAL/MOL/K  
 B= 0.000 C= 0.000  
 D= 0.000 E= 0.000  
 LIMIT= 1000.000 K  
 NO T-P DATA GRID  
 O SPECIES IN REACTION=  
 0.000 XX 0.000 XX 0.000 XX  
 LOG K= 500.000 DELHOR= 500.000 KCAL/MOL  
 DELSOR= 500.000 CAL/MOL/K  
 \* KIM (1983A) DETERMINED SOLUBILITY UNDER UNKNOWN REDOX CONDITIONS;  
 \* CANNOT RELATE TO AM+++ CONCENTRATION.  
 +-----  
 STOP.  
 MDSOLAM

#### DATA ON MINERALS AND RELATED SUBSTANCES OF AMERICIUM

NOTATION--  
 -- DELGO = GIBBS ENERGY OF FORMATION  
 -- DELGOR = GIBBS ENERGY OF REACTION  
 -- DELHO = ENTHALPY OF FORMATION  
 -- DELHOR = ENTHALPY OF REACTION  
 -- SO = CONVENTIONAL ENTROPY  
 -- DELSOR = ENTROPY OF REACTION

NOTE THAT "500." IS ENTERED TO MEAN "NO DATA" FOR DELGO, DELHO, SO,  
 DELHTR, DELSTR, LOG K, DELHO, AND DELSOR. NEVER ENTER ZERO FOR THESE  
 PARAMETERS OR LEAVE THEM BLANK UNLESS YOU MEAN TO USE AN ACTUAL VALUE OF  
 ZERO. 1000 K IS THE DEFAULT FOR THE "LIMIT" PARAMETER.

IONIC STRENGTH CORRECTIONS WERE MADE USING THE DAVIES EQUATION IN  
 THE FORM

$\text{LOG}(\text{GAMMA}) = 0.51 * (\text{Z}^{**2}) * (\text{SQR}(\text{I}) / (1 + \text{SQR}(\text{I}))) - (0.2 * \text{I})$   
 WHERE GAMMA IS THE ACTIVITY COEFFICIENT, Z IS THE CHARGE, AND  
 I IS THE IONIC STRENGTH.

#### DATA FOR SOLID/GAS SPECIES=

NAME= AN ALPHABETIC OR ALPHANUMERIC STRING; E.G., CALCITE, BISCHOFITE.  
 THE FORMULA MAY ALSO BE USED AS THE NAME.  
 FORMULA= AN ALPHANUMERIC STRING DENOTING THE FORMULA OF THE SPECIES;  
 E.G., CACO3, MGCL2.6H2O.  
 ENTERED BY= NAME OF PERSON WHO ENTERED DATA OR LAST REVISED IT  
 DATE= DATA OF ENTERING OR REVISING DATA  
 SOURCE= ALPHANUMERIC STRING IDENTIFYING A MAJOR SOURCE OF DATA. USE  
 "SEE BELOW" FOR MINOR SOURCES  
 QUALITY= ALPHANUMERIC STRING DESCRIBING THE PROBABLE ERROR IN GIBBS ENERGY  
 OR ITS EQUIVALENT, BASED ON SUBJECTIVE JUDGEMENT AND CHOSEN FROM  
 AMONG THE FOLLOWING (IN ORDER OF INCREASING VALUE)  
 BAD - DEMONSTRABLY BAD DATA- DO NOT USE EXCEPT IN ILLUSTRATIVE  
 CALCULATIONS  
 POOR - LIKELY ERROR EXCEEDS A COUPLE OF KCAL OR SEVERAL KJ  
 RESTRICTED - AD HOC FIT TO A PARTICULAR SITUATION; SEE NOTES  
 SPECULATIVE - SPECIES NOT SHOWN CONCLUSIVELY TO EXIST  
 UNCERTAIN - CHOSEN RATHER ARBITRARILY FROM DIVERGENT REPORTED  
 VALUES  
 UNSPECIFIED - NO QUALITY INFORMATION  
 (BLANK) - EQUIVALENT TO UNSPECIFIED  
 FAIR - LIKELY ERROR LESS THAN A COUPLE OF KCAL OR A FEW KJ  
 GOOD - LIKELY ERROR LESS THAN ABOUT ONE KCAL OR FOUR KJ  
 THE CODE MUST BE MODIFIED TO ALLOW OTHER QUALITY PARAMETER INPUTS.

UNRECOGNIZED INPUTS ARE SET TO "ERROR". DATA FOR WHICH THE QUALITY IS "RESTRICTED", "SPECULATIVE", OR "UNCERTAIN" MAY NUMERICALLY BE "FAIR" TO "GOOD". THE MAJOR UNCERTAINTY ASSOCIATED WITH THESE VALUES IS QUALITATIVE (I.E., UNCERTAINTY OF INTERPRETATION). DATA FOR WHICH THE QUALITY IS "POOR" MAY BE QUITE SUFFICIENT FOR MAKING "GOOD" CALCULATIONS- THIS DEPENDS ON THE SENSITIVITY OF THE RESULTS TO IT IN ANY PARTICULAR APPLICATION.

NUMBER OF CHEMICAL ELEMENTS PER MOLE

NUMBER OF MOLES OF ELEMENT PER MOLE OF SUBSTANCE

SYMBOL OF CHEMICAL ELEMENT

TEMP= THE BASE POINT TEMPERATURE (K), USUALLY 298.15 K

PRESS= THE BASE POINT PRESSURE (BARS), USUALLY 1 BAR

DELGO= THE APPARENT STANDARD PARTIAL MOLAL GIBBS ENERGY AT THE BASE POINT

DELHO= THE APPARENT STANDARD PARTIAL MOLAL ENTHALPY AT THE BASE POINT

SO= THE CONVENTIONAL ENTROPY AT THE BASE POINT

VO= THE MOLAR VOLUME AT THE BASE POINT

NUMBER OF HEAT CAPACITY RANGES THAT FOLLOW

EQUATION= HEAT CAPACITY EQUATION CODE

$$O - CP = A + 1.E-3*B*T + 1.E+5*C*T**(-2) + 1.E-6*D*T**2$$

$$1 - CP = A + 1.E-3*B*T + 1.E+5*C*T**(-2) + 1.E+8*D*T**(-3)$$

CP= THE MOLAR HEAT CAPACITY, ASSUMED TO BE A CONSTANT

A= FIRST HEAT CAPACITY COEFFICIENT

B= SECOND HEAT CAPACITY COEFFICIENT

C= THIRD HEAT CAPACITY COEFFICIENT

D= FOURTH HEAT CAPACITY COEFFICIENT

E= FIFTH HEAT CAPACITY COEFFICIENT

LIMIT= UPPER LIMIT (K) OF THE PRECEDING SET OF HEAT CAPACITY PARAMETERS;

NO T-P DATA GRID

THIS IS EITHER THE UPPER LIMIT OF USE BASED ON THE RANGE OF MEASUREMENT

OR THE TEMPERATURE OF A PHASE TRANSITION

DELHTR= ENTHALPY OF A PHASE TRANSITION, IF ANY

DELSTR= ENTROPY OF A PHASE TRANSITION, IF ANY

T-P DATA GRID INDICATION LINE, FOLLOWED BY T-P DATA GRID, IF ANY

TEMP, PRESS, DELGO, DELHO, SO, VO

NUMBER OF SPECIES APPEARING IN A REACTION, IF A REACTION FOLLOWS

NUMBER OF MOLES OF A SPECIES APPEARING IN THE REACTION

THE NAME OF THE CORRESPONDING SPECIES

LOG K= LOG OF THE EQUILIBRIUM CONSTANT OF THE GIVEN REACTION AT THE BASE POINT

DELHOR= ENTHALPY OF THE GIVEN REACTION AT THE BASE POINT

DELSOR= ENTROPY OF THE GIVEN REACTION AT THE BASE POINT

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STOP.

## APPENDIX C

Appendix C contains a listing of the input file REAC for the MCRT program. This file defines the chemical reactions of americium species that were considered.

RUN BY= J. F. KERRISK  
 DATE= 09/01/83  
 O O O O O O O O  
 AQUEOUS SPECIES OF AMERICIUM 8/03/83  
 AM+++ 1  
 1.00000 AM+++  
 AM++++ 5  
 -1.00000 AM++++  
 1.00000 H+  
 0.25000 O2(G)  
 AMO2+ 5  
 -1.00000 AMO2+  
 1.00000 H2O  
 0.50000 O2(G)  
 AMO2++ 5  
 -4.00000 AMO2++  
 2.00000 H2O  
 3.00000 O2(G)  
 AMOH++ 3  
 -1.00000 AMOH++  
 1.00000 OH-  
 AM(OH)2+ 3  
 -1.00000 AM(OH)2+  
 2.00000 OH-  
 AM(OH)3 3  
 -1.00000 AM(OH)3  
 3.00000 OH-  
 AMCO3+ 3  
 -1.00000 AMCO3+  
 1.00000 CO3--  
 AM(CO3)2- 3  
 -1.00000 AM(CO3)2-  
 2.00000 CO3--  
 AM(CO3)3--- 3  
 -1.00000 AM(CO3)3---  
 3.00000 CO3--  
 AM(OH)CO3 4  
 -1.00000 AM(OH)CO3  
 1.00000 OH-  
 AM(OH)2CO3- 4  
 -1.00000 AM(OH)2CO3-  
 2.00000 OH-  
 AM(OH)(CO3)2-- 4  
 -1.00000 AM(OH)(CO3)2--  
 1.00000 OH-  
 AMHC03++ 3  
 -1.00000 AMHC03++  
 1.00000 HC03-  
 AM(HC03)2+ 3  
 -1.00000 AM(HC03)2+  
 2.00000 HC03-  
 AMF++ 3  
 -1.00000 AMF++  
 1.00000 F-  
 AMF2+ 3  
 -1.00000 AMF2+  
 2.00000 F-  
 AMF3 3  
 -1.00000 AMF3  
 3.00000 F-  
 AMCL++ 3  
 -1.00000 AMCL++  
 1.00000 CL-  
 AMCL2+ 3  
 -1.00000 AMCL2+  
 2.00000 CL-  
 AMSO4+ 3  
 -1.00000 AMSO4+  
 1.00000 SO4--  
 AM(SO4)2- 3  
 -1.00000 AM(SO4)2-  
 2.00000 SO4--  
 AMH2PO4++ 3  
 -1.00000 AMH2PO4++  
 1.00000 H2PO4-  
 AM(H2PO4)2+ 3  
 -1.00000 AM(H2PO4)2+  
 2.00000 H2PO4-  
 AM(H2PO4)3 3  
 -1.00000 AM(H2PO4)3

3.00000 H <sub>2</sub> P <sub>O</sub> 4-		
AM(H <sub>2</sub> P <sub>O</sub> 4)4-	3	
- 1.00000 AM(H <sub>2</sub> P <sub>O</sub> 4)4-		1.00000 AM+++
4.00000 H <sub>2</sub> P <sub>O</sub> 4-		
AMN03++	3	
- 1.00000 AMN03++		1.00000 AM+++
1.00000 N03-		
AM(N03)2+	3	
- 1.00000 AM(N03)2+		1.00000 AM+++
2.00000 N03-		
AM02HC03	3	
- 1.00000 AM02HC03		1.00000 AM02+
1.00000 HC03-		
SOLIDS OF AMERICIUM		8/03/83
AM(OH)3(C)	3	
- 1.00000 AM(OH)3(C)		1.00000 AM+++
3.00000 OH-		
AM(OH)C03(C)	4	
- 1.00000 AM(OH)C03(C)		1.00000 AM+++
1.00000 OH-		1.00000 C03--
AM2(CD3)3(C)	3	
- 1.00000 AM2(CD3)3(C)		2.00000 AM+++
3.00000 CD3--		

STOP.

## APPENDIX D

Appendix D contains a listing of the output file DFILE from the MCRT program. This file contains the equilibrium-constant data for the reactions specified in Appendix C.

\*\*\*\*\* AQUEOUS \*\*\*\*\*

---

AM+++  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= GOOD  
 CHARGE= 3.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 8.0 A HYDR. NUMBER= 0.0  
 1 CHEMICAL ELEMENTS= 1.000 AM  
 1 SPECIES IN REACTION= 1.000 AM+++  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
     115.5310 104.9634 92.8252 81.7070  
     70.7079 61.9886 54.8845 48.9704  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
     0.0000 0.0000 0.0000 0.0000  
     0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSO.3230U02 , REV. 09/01/83, CRISS-COBBLE METHOD  
 \* (QUALITY OF AM+++ DATA = GOOD )

---

AM++++  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 4.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 11.0 A HYDR. NUMBER= 0.0  
 1 CHEMICAL ELEMENTS= 1.000 AM  
 5 SPECIES IN REACTION= -1.000 AM++++ -.500 H2O 1.000 H+  
     1.000 AM++ .250 O2(G)  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
     19.4620 18.8062 18.0343 17.3090  
     16.5681 15.9597 15.4548 15.0276  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
     0.0000 0.0000 0.0000 0.0000  
     0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, CRISS-COBBLE METHOD  
 \* (QUALITY OF AM++++ DATA = UNSPECIFIED )

---

AM02+  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 2 CHEMICAL ELEMENTS= 1.000 AM 2.000 O  
 5 SPECIES IN REACTION= -1.000 AM02+ -2.000 H+ 1.000 H2O  
     1.000 AM++ .500 O2(G)  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
     18.2750 16.7018 14.9026 13.2254  
     11.5162 10.1138 8.9127 7.8565  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
     0.0000 0.0000 0.0000 0.0000  
     0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, CRISS-COBBLE METHOD  
 \* (QUALITY OF AM02+ DATA = UNSPECIFIED )

---

AM02++  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 5.0 A HYDR. NUMBER= 0.0  
 2 CHEMICAL ELEMENTS= 1.000 AM 2.000 O  
 5 SPECIES IN REACTION= -4.000 AM02++ -4.000 H+ 2.000 H2O  
     4.000 AM++ 3.000 O2(G)  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
     98.2481 91.3093 83.3951 76.1488  
     68.9628 63.2418 58.5271 54.5462  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
     0.0000 0.0000 0.0000 0.0000  
     0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, CRISS-COBBLE METHOD  
 \* (QUALITY OF AM02++ DATA = UNSPECIFIED )

---

AMDH++  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED

CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 5.0 A HYDR. NUMBER= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 1.000 O 1.000 H  
 3 SPECIES IN REACTION=  
 -1.000 AMOH++ 1.000 AM+++ 1.000 OH-  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -7.5615 -7.5615 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AMOH++) DATA = UNSPECIFIED )  
 +-----  
**AM(OH)2+**  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 2.000 O 2.000 H  
 3 SPECIES IN REACTION=  
 -1.000 AM(OH)2+ 1.000 AM+++ 2.000 OH-  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -13.7009 -13.7009 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM(OH)2+) DATA = UNSPECIFIED )  
 +-----  
**AM(OH)3**  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 0.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 3.000 O 3.000 H  
 3 SPECIES IN REACTION=  
 -1.000 AM(OH)3 1.000 AM+++ 3.000 OH-  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -18.8802 -18.8802 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM(OH)3) DATA = UNSPECIFIED )  
 +-----  
**AMCO3+**  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 3.000 O 1.000 CO3--  
 3 SPECIES IN REACTION=  
 -1.000 AMCO3+ 1.000 AM+++ 1.000 CO3--  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -7.6524 -7.6524 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AMCO3+) DATA = UNSPECIFIED )  
 +-----  
**AM(CO3)2-**  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= -1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 6.000 O 2.000 CO3--  
 3 SPECIES IN REACTION=  
 -1.000 AM(CO3)2- 1.000 AM+++ 2.000 CO3--  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -12.1675 -12.1675 500.0000 500.0000

\* 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 \* 0.0000 0.0000 0.0000 0.0000  
 \* 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM(CO3)2- DATA = UNSPECIFIED )  
 +-----  
 AM(CO3)3---  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= -3.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 3.000 C 9.000 D  
 3 SPECIES IN REACTION=  
 -1.000 AM(CO3)3--- 1.000 AM+++ 3.000 CO3--  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 \* 500.0000 500.0000 500.0000 500.0000  
 \* 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 \* 0.0000 0.0000 0.0000 0.0000  
 \* 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM(CO3)3--- DATA = UNSPECIFIED )  
 +-----  
 AM(OH)CO3  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 0.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 4 CHEMICAL ELEMENTS=  
 1.000 AM 4.000 O 1.000 H  
 1.000 C  
 4 SPECIES IN REACTION=  
 -1.000 AM(OH)CO3 1.000 AM+++ 1.000 OH-  
 1.000 CO3--  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 \* 500.0000 500.0000 500.0000 500.0000  
 \* 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 \* 0.0000 0.0000 0.0000 0.0000  
 \* 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM(OH)CO3 DATA = UNSPECIFIED )  
 +-----  
 AM(OH)2CO3-  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= -1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 4 CHEMICAL ELEMENTS=  
 1.000 AM 5.000 D 2.000 H  
 1.000 C  
 4 SPECIES IN REACTION=  
 -1.000 AM(OH)2CO3- 1.000 AM+++ 2.000 OH-  
 1.000 CO3--  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 \* 500.0000 500.0000 500.0000 500.0000  
 \* 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 \* 0.0000 0.0000 0.0000 0.0000  
 \* 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM(OH)2CO3- DATA = UNSPECIFIED )  
 +-----  
 AM(OH)(CO3)2--  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= -2.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 4 CHEMICAL ELEMENTS=  
 1.000 AM 1.000 H 7.000 O  
 2.000 C  
 4 SPECIES IN REACTION=  
 -1.000 AM(OH)(CO3)2 1.000 AM+++ 1.000 OH-  
 2.000 CO3--  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 \* 500.0000 500.0000 500.0000 500.0000  
 \* 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =

0.0000 0.0000 0.0000 0.0000  
0.0000 0.0000 0.0000 0.0000  
\* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
\* (QUALITY OF AM(OH)(CO3)2-- DATA = UNSPECIFIED )

+-----  
AMHC03++  
ENTERED BY= J. F. KERRISK DATE= 09/01/83  
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL  
ION SIZE= 5.0 A HYDR. NUMBER= 0.0  
4 CHEMICAL ELEMENTS=  
1.000 AM 1.000 H 1.000 C  
3.000 D  
3 SPECIES IN REACTION=  
-1.000 AMHC03++ 1.000 AM+++ 1.000 HC03-  
\* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
500.0000 500.0000 500.0000 500.0000  
500.0000 500.0000 500.0000 500.0000  
\* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
0.0000 0.0000 0.0000 0.0000  
0.0000 0.0000 0.0000 0.0000  
\* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
\* (QUALITY OF AMHC03++) DATA = UNSPECIFIED )

+-----  
AM(HC03)2+  
ENTERED BY= J. F. KERRISK DATE= 09/01/83  
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
4 CHEMICAL ELEMENTS=  
1.000 AM 2.000 H 2.000 C  
6.000 D  
3 SPECIES IN REACTION=  
-1.000 AM(HC03)2+ 1.000 AM+++ 2.000 HC03-  
\* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
500.0000 500.0000 500.0000 500.0000  
500.0000 500.0000 500.0000 500.0000  
\* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
0.0000 0.0000 0.0000 0.0000  
0.0000 0.0000 0.0000 0.0000  
\* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
\* (QUALITY OF AM(HC03)2+) DATA = UNSPECIFIED )

+-----  
AMF++  
ENTERED BY= J. F. KERRISK DATE= 09/01/83  
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL  
ION SIZE= 5.0 A HYDR. NUMBER= 0.0  
2 CHEMICAL ELEMENTS=  
1.000 AM 1.000 F  
3 SPECIES IN REACTION=  
-1.000 AMF++ 1.000 AM+++ 1.000 F-  
\* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
-4.2246 -4.3004 -4.4779 -4.7507  
-5.1725 -5.6792 -6.3105 -7.1899  
\* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
0.0000 0.0000 0.0000 0.0000  
0.0000 0.0000 0.0000 0.0000  
\* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, CRISS-COBBLE METHOD  
\* (QUALITY OF AMF++) DATA = UNSPECIFIED )

+-----  
AMF2+  
ENTERED BY= J. F. KERRISK DATE= 09/01/83  
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
2 CHEMICAL ELEMENTS=  
1.000 AM 2.000 F  
3 SPECIES IN REACTION=  
-1.000 AMF2+ 1.000 AM+++ 2.000 F-  
\* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
-7.3987 -7.3987 500.0000 500.0000  
500.0000 500.0000 500.0000 500.0000  
\* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
0.0000 0.0000 0.0000 0.0000  
0.0000 0.0000 0.0000 0.0000  
\* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
\* (QUALITY OF AMF2+) DATA = UNSPECIFIED )

+-----  
AMF3

ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 0.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 2 CHEMICAL ELEMENTS=  
 1.000 AM 3.000 F  
 3 SPECIES IN REACTION=  
 -1.000 AMF3 1.000 AM+++ 3.000 F-  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -10.5997 -10.5997 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AMF3 DATA = UNSPECIFIED )  
 +-----  
 AMCL++  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 5.0 A HYDR. NUMBER= 0.0  
 2 CHEMICAL ELEMENTS=  
 1.000 AM 1.000 CL  
 3 SPECIES IN REACTION=  
 -1.000 AMCL++ 1.000 AM+++ 1.000 CL-  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -1.0995 -1.0995 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AMCL++ DATA = UNSPECIFIED )  
 +-----  
 AMCL2+  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 2 CHEMICAL ELEMENTS=  
 1.000 AM 2.000 CL  
 3 SPECIES IN REACTION=  
 -1.000 AMCL2+ 1.000 AM+++ 2.000 CL-  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -1.5613 -1.5613 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AMCL2+ DATA = UNSPECIFIED )  
 +-----  
 AMSO4+  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 4.000 O 1.000 S  
 3 SPECIES IN REACTION=  
 -1.000 AMSO4+ 1.000 AM+++ 1.000 SO4--  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -3.5982 -3.5982 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AMSO4+ DATA = UNSPECIFIED )  
 +-----  
 AM(SO4)2-  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= -1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 8.000 O 2.000 S  
 3 SPECIES IN REACTION=  
 -1.000 AM(SO4)2- 1.000 AM+++ 2.000 SO4--

```

* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-4.9975 -4.9975 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AM(SO4)2- DATA = UNSPECIFIED )
+-----+
AMH2PO4++
ENTERED BY= J. F. KERRISK DATE= 09/01/83
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 5.0 A HYDR. NUMBER= 0.0
4 CHEMICAL ELEMENTS=
1.000 AM 4.000 D 1.000 P
2.000 H
3 SPECIES IN REACTION=
-1.000 AMH2PO4++ 1.000 AM+++ 1.000 H2PO4-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-2.7267 -2.7267 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AMH2PO4++ DATA = UNSPECIFIED )
+-----+
AM(H2PO4)2+
ENTERED BY= J. F. KERRISK DATE= 09/01/83
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 4.0 A HYDR. NUMBER= 0.0
4 CHEMICAL ELEMENTS=
1.000 AM 8.000 D 2.000 P
4.000 H
3 SPECIES IN REACTION=
-1.000 AM(H2PO4)2+ 1.000 AM+++ 2.000 H2PO4-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-3.7162 -3.7162 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AM(H2PO4)2+ DATA = UNSPECIFIED )
+-----+
AM(H2PO4)3
ENTERED BY= J. F. KERRISK DATE= 09/01/83
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
CHARGE= 0.0 TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 4.0 A HYDR. NUMBER= 0.0
4 CHEMICAL ELEMENTS=
1.000 AM 12.000 D 3.000 P
6.000 H
3 SPECIES IN REACTION=
-1.000 AM(H2PO4)3 1.000 AM+++ 3.000 H2PO4-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-4.6911 -4.6911 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =
0.0000 0.0000 0.0000 0.0000
0.0000 0.0000 0.0000 0.0000
* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA
* (QUALITY OF AM(H2PO4)3 DATA = UNSPECIFIED )
+-----+
AM(H2PO4)4-
ENTERED BY= J. F. KERRISK DATE= 09/01/83
SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED
CHARGE= -1.0 TITR. FACTOR= 0.0 EQ/MOL
ION SIZE= 4.0 A HYDR. NUMBER= 0.0
4 CHEMICAL ELEMENTS=
1.000 AM 16.000 D 4.000 P
8.000 H
3 SPECIES IN REACTION=
-1.000 AM(H2PO4)4- 1.000 AM+++ 4.000 H2PO4-
* LOG K GRID (0-25-60-100/150-200-250-300 C) =
-5.2408 -5.2408 500.0000 500.0000
500.0000 500.0000 500.0000 500.0000
* DELVR GRID (0-25-60-100/150-200-250-300 C) =

```

0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM(H2PO4)4- DATA = UNSPECIFIED )  
 +-----  
 AMNO3++  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 2.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 5.0 A HYDR. NUMBER= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 3.000 O 1.000 N  
 3 SPECIES IN REACTION=  
 -1.000 AMNO3++ 1.000 AM+++ 1.000 NO3-  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -1.1515 -1.1515 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AMNO3++) DATA = UNSPECIFIED )  
 +-----  
 AM(NO3)2+  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 1.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 6.000 O 2.000 N  
 3 SPECIES IN REACTION=  
 -1.000 AM(NO3)2+ 1.000 AM+++ 2.000 NO3-  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -1.6580 -1.6580 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM(NO3)2+) DATA = UNSPECIFIED )  
 +-----  
 AM02HC03  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 CHARGE= 0.0 TITR. FACTOR= 0.0 EQ/MOL  
 ION SIZE= 4.0 A HYDR. NUMBER= 0.0  
 4 CHEMICAL ELEMENTS=  
 1.000 AM 1.000 H 1.000 C  
 5.000 O  
 3 SPECIES IN REACTION=  
 -1.000 AM02HC03 1.000 AMD2+ 1.000 HC03-  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -2.3001 -2.3001 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDAQSAM DATA F, REV. 10/04/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM02HC03) DATA = UNSPECIFIED )  
 +-----  
 \*\*\*\* SOLIDS \*\*\*\*=  
 +-----  
 AM(OH)3(C)  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 VOLUME= 0.000 CC/MOL  
 3 CHEMICAL ELEMENTS=  
 1.000 AM 3.000 O 3.000 H  
 3 SPECIES IN REACTION=  
 -1.000 AM(OH)3(C) 1.000 AM+++ 3.000 OH-  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -27.8006 -27.8006 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDSOLAM DAT, REV. 10/03/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM(OH)3(C)) DATA = UNSPECIFIED )  
 +-----  
 AM(OH)C03(C)

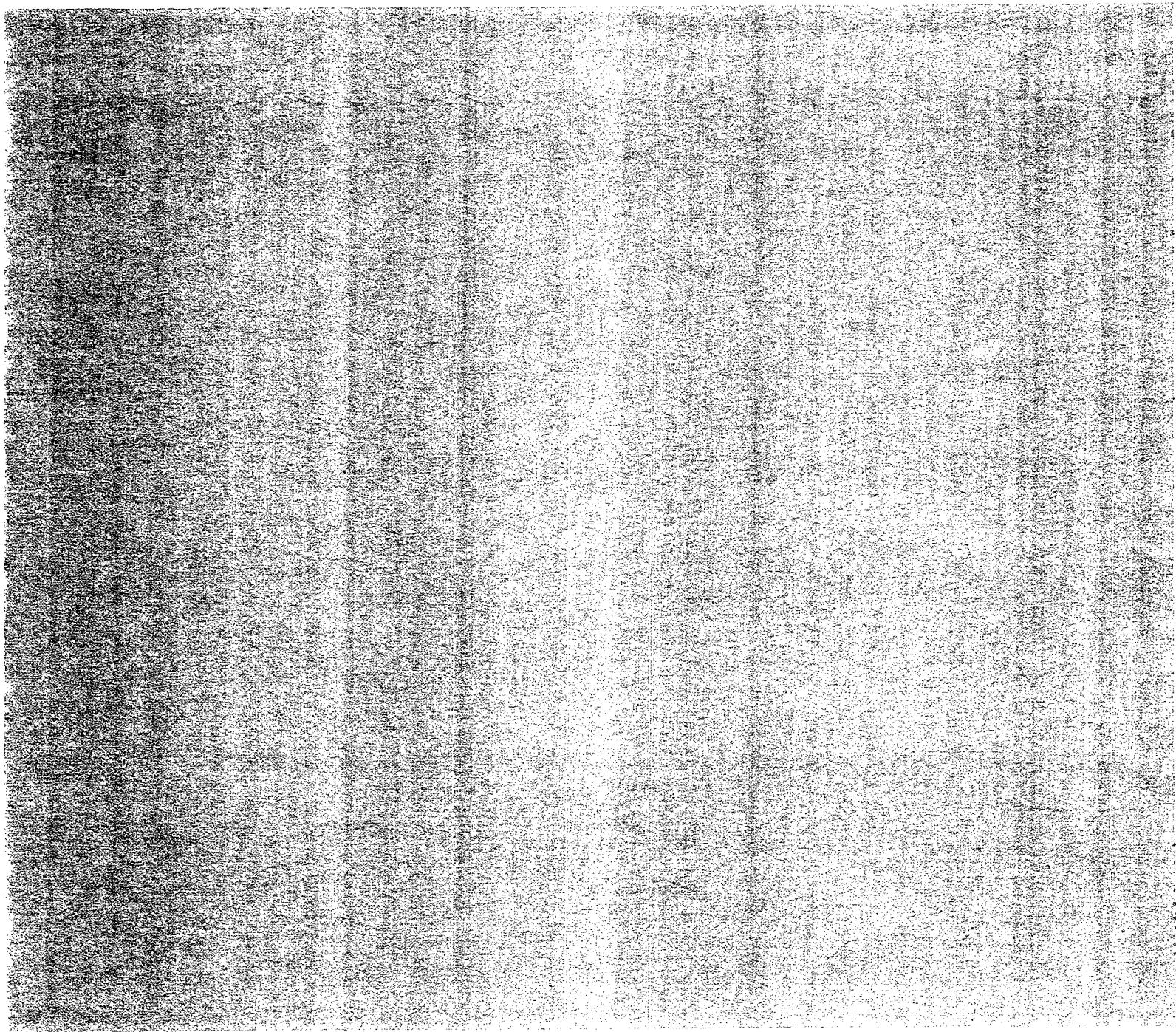
ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 VOLUME= 0.000 CC/MOL  
 4 CHEMICAL ELEMENTS=  
 1.000 AM 1.000 C 1.000 H  
 4.000 O  
 4 SPECIES IN REACTION=  
 -1.000 AM(OH)CO3(C) 1.000 AM+++ 1.000 OH-  
 1.000 CO3--  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -22.7709 -22.7709 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDSOLAM DAT, REV. 10/03/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM(OH)CO3(C) DATA = UNSPECIFIED )  
 +-----  
 AM2(CO3)3(C)  
 ENTERED BY= J. F. KERRISK DATE= 09/01/83  
 SOURCE= MCRT.3230U03 QUALITY= UNSPECIFIED  
 VOLUME= 0.000 CC/MOL  
 3 CHEMICAL ELEMENTS=  
 2.000 AM 3.000 C 9.000 O  
 3 SPECIES IN REACTION=  
 -1.000 AM2(CO3)3(C) 2.000 AM+++ 3.000 CO3--  
 \* LOG K GRID (0-25-60-100/150-200-250-300 C) =  
 -37.5215 -37.5215 500.0000 500.0000  
 500.0000 500.0000 500.0000 500.0000  
 \* DELVR GRID (0-25-60-100/150-200-250-300 C) =  
 0.0000 0.0000 0.0000 0.0000  
 0.0000 0.0000 0.0000 0.0000  
 \* MCRT FILE MDSOLAM DAT, REV. 10/03/83, INSUFFICIENT DATA  
 \* (QUALITY OF AM2(CO3)3(C) DATA = UNSPECIFIED )  
 +-----

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